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In this study we have re-analyzed high-resolution spectra of pure CO and CO broadened by hydrogen recorded in the spectral range of the first overtone band [1]. Self- and H_2-Lorentzian pressure-broadened half-width, pressure-induced shift parameters, line mixing coefficients as well as line centers and intensities were obtained for 48 (P(24) to R(23)) ro-vibrational transitions belonging to the first overtone (2←0) band of $^{12}C^{16}O$ at the ambient temperature (~298 K).

The diffusion constants needed to estimate the narrowing line parameters were calculated theoretically. H_2 was modeled by means of a single united atom force field [2] while CO was described from a three electrostatic sites model [3]. Intermolecular interactions were described by combining electrostatic and van der Waals interactions. The electrostatic contribution was computed using the Ewald sum while the van der Waals interactions were modeled from a Lennard-Jones potential. For CO-H_2 mixtures, five molar fractions were investigated, 0.0, 0.0126, 0.05, 0.5 and 1. Molecular dynamics simulations were carried out using the DLPOLY software [4]. This procedure allowed us to fix the narrowing parameters to the calculated values while fitting the spectra with the Rautian and speed-dependent Rautian profiles.

The spectra were fitted simultaneously within the range 4146 to 4332 cm^{-1} employing four line shape functions: the Voigt, Speed Dependent Voigt, Rautian and Speed Dependent Rautian Profiles. The line coupling effect has been observed and investigated as an asymmetry in the analyzed line profiles. Two semi-empirical methods (Energy Corrected Sudden Approximation, Exponential Power Gap Law) were used to estimate the self-broadening and self-line mixing parameters.
Furthermore, a classical approach [5] was applied to calculate the half-widths of CO absorption lines in CO-H_2 and CO-CO collisions. The calculations utilize simple vibrationally independent intermolecular interaction potential (Tipping-Herman + electrostatic) [6,7]. Both molecules were treated as rigid rotors. The dependences of CO half-widths on rotational quantum number for $J \leq 24$ are computed at room temperature and compared with measured data.

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